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Our results for the singlet case are reported shows that the singlet case is more problematic, as the existing theories are not all in agreement. Since the GHF is quite distinct from all the other approaches and based on the potentially powerful SCF approach, further analyses should help clarify the situation.

A part of our study in progress includes an extension of additional channels in the total wave function to test the convergence of the theory. We adopt a vartiational procedure to improve on the ionization differential cross section. This work will be reported elsewhere.

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I. Introduction

In view of the successful application of the Hartree-Fock approach to many-particle bound state problems in the past, we have attempted a similar treatment for the scattering systems. The conventional theories which have been used in the past for the bound state problems are not quite applicable for scattering and ionization problems, mainly because there are one or more continuum wave functions involved in the description of the final states. Evidently, the continuum functions are not square-integrable i.e. not L2, and this fact complicates the mathematical as well as the computational aspect of the theory. In order to remove this fundamental difficulty, we have developed a new procedure that introduces an amputation of the scattering function at large distance, making it square-integrable. Note that, except for the phase shift, the tail of the continuum function carries minimal dynamic information. The use of the amputated functions thus allowed the development of a self-consistent procedure for the evaluation of the scattering amplitude in a systematic way. It is termed a generalized Hartree-Fock theory (GHF).

In the present work, we extend the GHF theory to the ionization problem, where at least two continuum functions are to be made square-integrable (L2) by the amputation procedure. As the GHF theory focuses on properly treating the continuum function, it is eminently suited for the ionization problem. As preliminary to a full treatment of many physically interesting cases, we study in this report a simple electron-hydrogen scattering in the zero angular momentum approximation. Although the angular momentum is uncoupled, this model problem still contains much of the difficulties of a three-body Coulomb problem, and it also serves as a non-trivial test of the new approach to the ionization problem. In section II the GHF theory for the elastic scattering is extended to the ionization process. Our results are summarized in Sec. III.

II. Ionization by electron impact

The GHF for scattering summarized above can immediately be adapted to the ionization problem of interest here in a natural way, because the amputation can now be carried out on the two continuum functions. The final state wave function is written as

$$\Psi = A\Psi_{-k-p}\,\varphi_k\,\varphi_p$$

where Ψ_{-k-p} is the residual target function of N-2 electrons and φ_k, φ_p are the continuum functions. The amputation is then carried out simply as

$$X_k = D_k\,\varphi_k \quad \text{and} \quad X_p = D_p\,\varphi_p$$

where D_k and D_p may be different , not only in the constant kinetic energies, but also possibly due to the presence of long-range interaction. In some cases, the Coulomb potentials may not be completely screened for the residual ions.
The transition amplitude T_{fi} is given by

$$T_{fi} = \left\langle \Psi_f \middle| H - E_t \middle| \Psi_i^{\,0} \right\rangle \quad ,$$

Ψ_f and $\Psi_i^{\,0}$ represent the wave functions describing the whole system in its fully interacting final state and non-interacting initial state, respectively. The fully differential cross section is given by

$$\frac{d\sigma}{d\hat{k}_1 d\hat{k}_2 d\varepsilon} = (2\pi)^4 \frac{k_1 k_2}{k} \left| T_{fi} \right|^2 \quad ,$$

As in the Hartree-Fock case, the resulting system of mutually coupled SCF equations is solved by iteration, subject to the self consistency requirement. First one guesses a set of scattering wave functions. Then one computes the SCF potentials and the inhomogeneous terms. The set of equations is then solved. These new scattering wave functions are amputated and used to compute the new SCF potentials and the new inhomogeneous terms, which in turn are used to obtain a third set of scattering wave functions. The cycle continues until self consistency is reached within some preset tolerance. The numerical method we adopt for the scattering functions is the use of the distorted Green's functions. In this method, we transform the set of differential equations that the scattering functions satisfy, along with their corresponding boundary conditions, into integral equations. The final step in the numerical procedure is to calculate the proper integral expressions for the scattering amplitudes T_{fi} and the corresponding ionization cross section.

III. Results

We first choose the GHF wave function of the scattering system, as in the case of Hartree-Fock, in its lowest approximation: $\Psi_{GHF} = \Psi_{GHF}^{\,0}$. We carried out calculations at total energies $E_t = 2.0\ Ry$ and $E_t = 3.0\ Ry$, since the previous data are available for these energies for comparison. Our results for the triplet case are reported in Table 1 and compared with the exterior complex scaling (ECS) method. The ECS method seems to be the most accurate procedure available for computing ionization cross section for the model. It uses a two-dimensional grid to solve for the outgoing scattered wave function without explicitly imposing the asymptotic boundary condition for the three charged particles. The coordinates are then scaled by a complex phase factor, beyond a certain radius where the tail of the Coulomb potential is ignored. As a result, the scattered wave

function decays like a bound state wave function, which makes the asymptotic boundary condition simple to satisfy. Figure 1 contains additional data obtained by the CCC. Agreement between our results and all the others is very good for the triplet case. This is especially surprising because the GHF approximation is considered here only in its lowest approximation. Apparently, the amputated wave functions carry much of the essential dynamical information contained in the scattering functions. Hence, we have been able to impose self consistency as a result of the amputation procedure which carefully gets rid of the long range tail represented by the asymptotic part of the scattering functions. Another feature of the GHF approach is that, by definition, our ionization differential cross sections are symmetric about the point $\frac{\varepsilon}{E} = 0.5$. This property is absent in the close-coupling approach.

In Figure 2 we display the interaction potential V^{GHF} between the two continuum electrons. This is the first time the SCF potential is displayed in the ionization problem. It is then compared to the pure Coulombic potential V^{C}. Figure 3 shows that the amputated wave function X which carries all the dynamics is of short range. It is presumably due to the character of the present model.

Our results for the singlet case are reported in Table 2. Figure 4 shows that the singlet case is more problematic, as the existing theories are not all in agreement. Since the GHF is quite distinct from all the other approaches and based on the potentially powerful SCF approach, further analyses should help clarify the situation.

A part of our study in progress includes an extension of additional channels in the total wave function to test the convergence of the theory. We adopt a vartiational procedure to improve on the ionization differential cross section. This work will be reported elsewhere.

V. Discussion

The present study shows that the GHF approach is a viable method to treat complex collision systems. The effectiveness of the theory may be attributed to the crucial physics information carried by the amputated wave function. It is possible in principle to obtain accurate solutions to the collision problem by adopting a "proper projection" of the scattering equations, although it is in general difficult to find the proper projection. However, the GHF seems to provide a partial answer to the projection problem, in terms of the amputated functions *X*. For application of GHF to more realistic and complex systems, it is important to better understand the role played by the *X*'s. The multiconfiguration extension of the GHF is in progress to clarify the situation.

Table 1. Single-differential ionization cross sections $\frac{d\sigma}{d\varepsilon}$ (in units of $\pi a_0^{\,2}$ / hartree) of e-H scattering system at $E = 2\ Ry$ and $3\ Ry$ are given as a function of the energy fraction $\frac{\varepsilon}{E}$ for S = 1 case where $E = E_1^{\,2} + E_2^{\,2} = \varepsilon + (E - \varepsilon)$. The Exterior Complex Scaling is denoted by *ECS* and the Generalized Hartree-Fock approach is denoted by *GHF*.

$\frac{\varepsilon}{E}$	$\frac{d\sigma}{d\varepsilon}^{ECS}(E = 2\,Ry)$	$\frac{d\sigma}{d\varepsilon}^{GHF}(E = 2\,Ry)$	$\frac{d\sigma}{d\varepsilon}^{ECS}(E = 3\,Ry)$	$\frac{d\sigma}{d\varepsilon}^{GHF}(E = 3\,Ry)$
0.15	0.00711	0.00782	0.00567	0.0073
0.175	0.00582	0.00607	0.00459	0.00556
0.2	0.00472	0.00474	0.00368	0.00420
0.225	0.00377	0.00371	0.00292	0.00315
0.25	0.00297	0.00289	0.00229	0.00235
0.275	0.00223	0.00224	0.00176	0.00173
0.3	0.00173	0.00171	0.00132	0.00125
0.325	0.00126	0.00128	0.00096	0.00089
0.35	0.00089	0.00092	0.00067	0.00061
0.375	0.00059	0.00063	0.00045	0.00041

0.4	0.00036	0.00040	0.00027	0.00025
0.425	0.00019	0.00022	0.00015	0.00014
0.45	0.00008	0.00009	0.00006	0.00006
0.475	0.00002	0.00002	0.0002	0.00002
0.5	0	0	0	0

Table 2. Single-differential ionization cross sections $\frac{d\sigma}{d\varepsilon}$ (in units of $\pi a_0^{\,2}$ / hartree) of e-H scattering system at $E = 2\ Ry$ and $3\ Ry$ are given as a function of the energy fraction $\frac{\varepsilon}{E}$ for the S = 0 case. The Exterior Complex Scaling is denoted by *ECS* and the Generalized Hartree-Fock approach is denoted by *GHF*.

$\frac{\varepsilon}{E}$	$\frac{d\sigma}{d\varepsilon}^{ECS}$ $(E = 2\,Ry)$	$\frac{d\sigma}{d\varepsilon}^{GHF}$ $(E = 2\,Ry))$	$\frac{d\sigma}{d\varepsilon}^{ECS}$ $(E = 3Ry)$	$\frac{d\sigma}{d\varepsilon}^{GHF}$ $(E = 3\,Ry)$
0.15	0.04542	0.04263	0.02278	0.02648
0.175	0.04387	0.03903	0.0218	0.02362
0.2	0.04242	0.03527	0.0209	0.02076
0.225	0.04103	0.03174	0.02008	0.0179
0.25	0.03969	0.02861	0.01932	0.01504
0.275	0.03838	0.02587	0.01861	0.01361
0.3	0.03709	0.02348	0.01793	0.01215
0.325	0.03581	0.02137	0.01728	0.01085
0.35	0.03453	0.01949	0.01665	0.00969
0.375	0.03323	0.01788	0.01603	0.00866
0.4	0.03192	0.01656	0.01543	0.00775
0.425	0.03063	0.01545	0.01484	0.00694

0.45	0.0294	0.01448	0.01428	0.00622
0.475	0.02838	0.01367	0.01383	0.00559
0.5	0.02792	0.01307	0.01362	0.00506

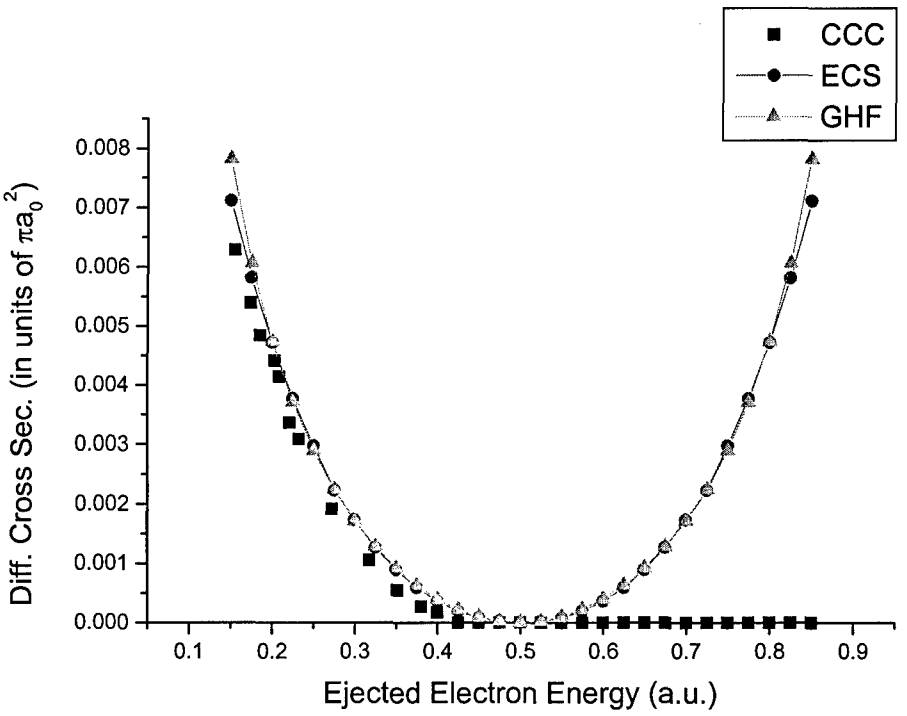
CCC
ECS
GHF
Diff. Cross Sec. (in units of πa_0^2)
0.000
0.001
0.002
0.003
0.004
0.005
0.006
0.007
0.008
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
Ejected Electron Energy (a.u.)

Figure 1

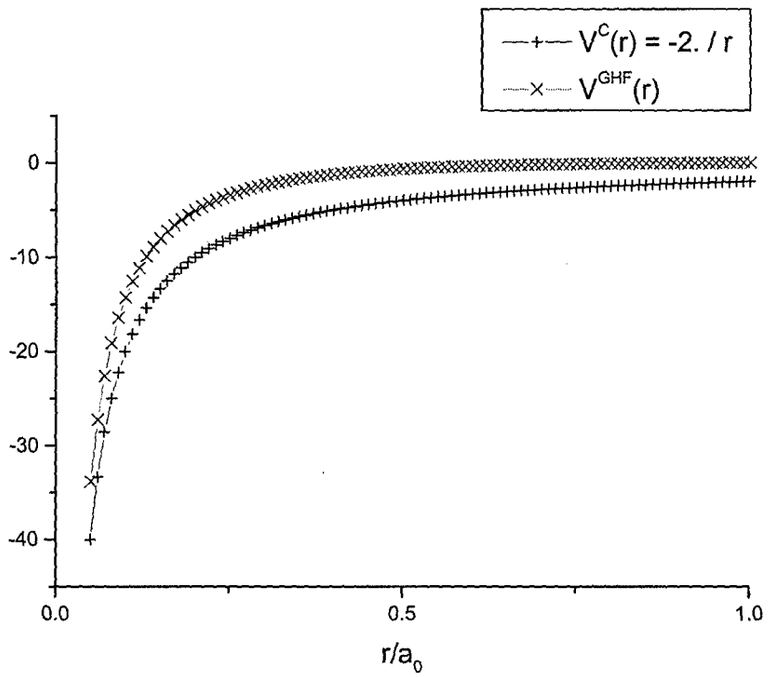

Figure 2

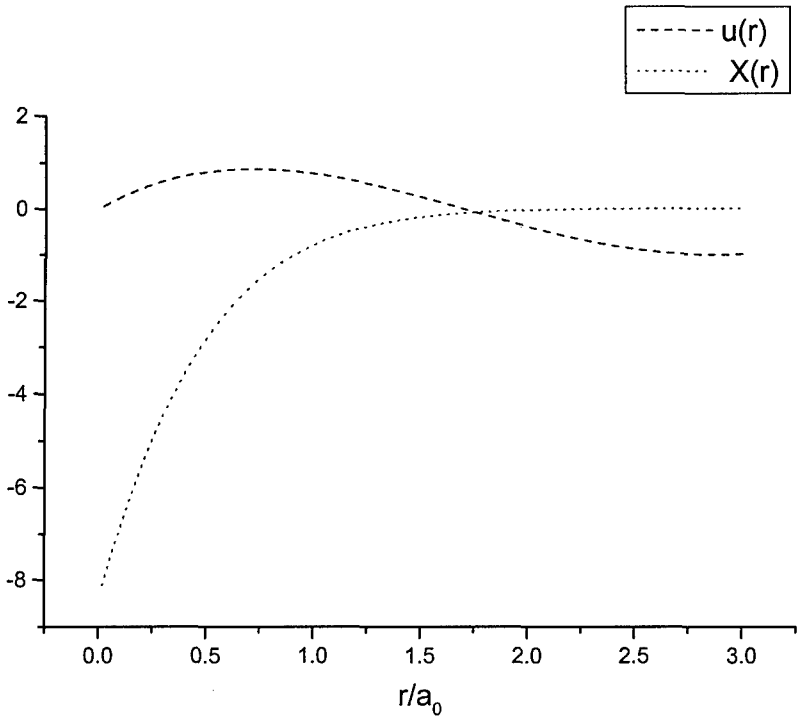

Figure 3

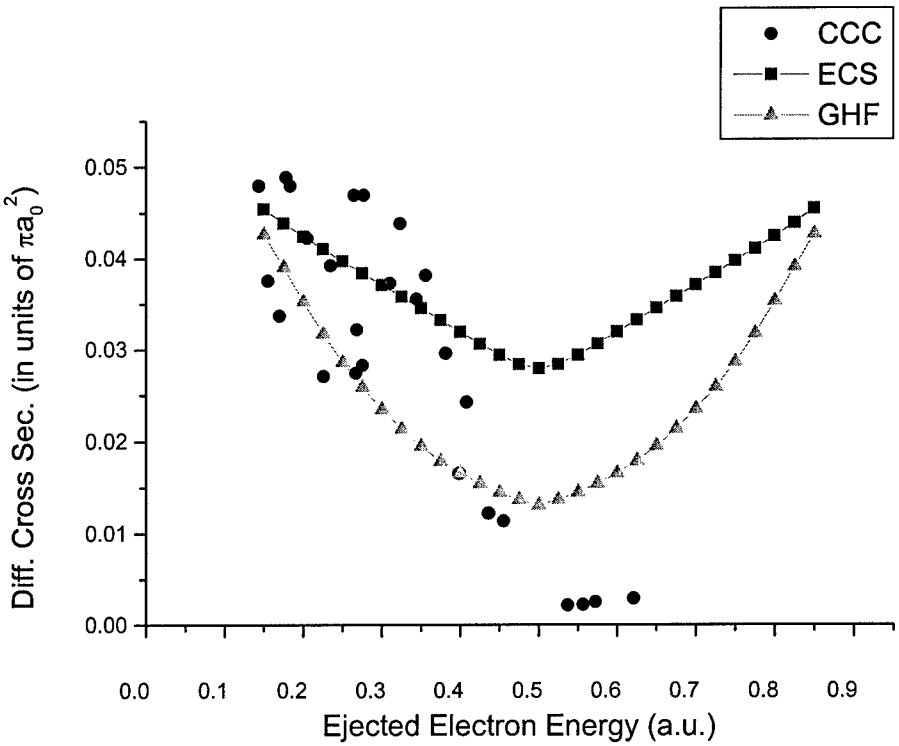
CCC
ECS
GHF
Diff. Cross Sec. (in units of πa_0^2)
0.05
0.04
0.03
0.02
0.01
0.00
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
Ejected Electron Energy (a.u.)

Figure 4